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Jeremy K. Burdett Department of Chemistry The University of Chicago Chicago, Illinois 60637 Contract N-00014-85-K-0354

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This annual report covers the period from April 15, 1925 to April 14, 1986. The report includes two technical reports on completed work which are being sent out to those on the distribution list as required.

The numerical work during the year has concentrated on two aspects of solids (i) seeing how well the pseudopotential approach developed by Chelikowsky and Louie works in getting the correct structure for simple solids and trying to understand why, as one moves across a pseudopotential structure map the statle structure changes. This work has now been published as a Physical Review Letter (Technical Report #1), (ii) Examination of the electronic band structures of some simple solids using less accurate methods in order to see how the substitution of Si for P or P for S in binary or ternary systems changes the details of the electronic structure and the relevant bond gaps. This work is in progress and represents the introduction to the solid state for a new postdoctoral.

In qualitative terms we have used the aspects of pseudcpotential radii to plot structure maps for ternary materials. Their use does allow a superior sorting compared to the ionic radii but is not particularly startling (Technical Report #2). We have had less success in correlating properties with the d/or pseudopotential radii due entirely to the lack of a sufficiently large database of properties.

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